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1  ##### 非階層クラスター分析#####
2  library(MASS)
3  data(Cars93 )
4  str(Cars93) #data構造:型, サンプルサイズ, 変数の数と内容
5  #####欠測値処理
6  anyNA(Cars93[, c(5, 7, 12:14, 17:19, 25)]) #指定範囲の項目にNAがあるか
7
8  #####Kmeans: 非階層クラスター分析の問題点: CLボリュームが初期値に依存, 最適CL数不明
9  ##CL数探索
10 #NbClust関数
11 library(NbClust)
12 w.cln <- NbClust(Cars93[, c(5, 7, 12, 14, 19, 22, 25)],
13                         min.nc = 2 , max.nc = 10,
14                         diss = NULL, distance = "euclidean",
15                         method = "kmeans", index="all", alphaBeale=0.1)
16 w.cln$Best.nc
17 par(mfrow=c(1, 1))
18 barplot(table(w.cln$Best.nc[1,]))
19 #####Within groups sum of squares:[R IN ACTION ],P.379-380から引用
20 d <- data.frame(scale(Cars93[,c(5, 7, 12, 14, 19, 22, 25)]))
21 cd <- scale(d)
22 set.seed(123)
23 wssplot <- function(data, nc=10 ){
24   wss2 <- (nrow(data)-1)*sum(apply(data, 2, var))
25   for (i in 2:nc){
26     wss2[i] <- sum(kmeans(data, centers=i)$withinss)}
27   plot(1:nc, wss2, type = "b", pch = 17 , lwd = 2,
28       xlab="Number of Clusters", ylab="Within groups sum of squares")}
29 wssplot(d)
30 wssplot(cd) #標準化data
31
32 ##### Kmeans #####
33 set.seed(123) #seedを指定しておくと再現性がある
34 kms <- kmeans(x = Cars93[,c(5, 7, 12, 14, 19, 22, 25)],
35                 centers = 3 ,           #centers=CL数の場合重心の初期値はランダム
36                 iter.max = 100 ,
37                 algorithm = c("Hartigan-Wong", "Lloyd",
38                               "Forgy", "MacQueen"), #4種類,省略可
39                 nstart = 1)           #centers=CL数の場合:選択すべきrandom sets数
40 names(kms)
41 kms
42 ##Fit
43 ss <- function(x) sum(scale(Cars93[,c(5, 7, 12, 14, 19, 22, 25)], scale = F)^2)
44 fitted.x <- fitted(kms); head(fitted.x)
45 resid.x <- Cars93[,c(5, 7, 12, 14, 19, 22, 25)] - fitted(kms)
46 resid.x
47 round(kms$betweens/kms$totss , 3)*100
48
49 #####CLを決めて元dataに書き込む: kmcl$cluster
50 km.cl <- factor(kms$cluster)
51 write.csv(cbind(Cars93 , data.frame(km.cl) ),
52           "data/cars93.cl.csv") #CLdata書き込み
53
54 #####Plot:多次元dataを2次元に縮約(Use PCA)
55 library(useful)
56 plot(data = Cars93[,c(5, 7, 12, 14, 19, 22, 25)] , kms )
57 library(cluster)
58 clusplot(Cars93[,c(5, 7, 12:14, 17:19, 25)],
59           kms$cluster, color = T, shade = F,
60           labels = 2, lines = 0)

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60
61 #####kmeans++(kmeanpp()関数)#####
62 #K-meansは初期重心をランダム配置するため近くに配置されることがあるがそれを避ける
63 #最初に1点を選択、結果を利用して重心を再配置(その後は通常のk-means)
64 install.packages("LICORS")
65 library(LICORS)
66 library(cluster)
67 library(RColorBrewer)
68 library(MASS)
69 data("Cars93")
70 str(Cars93)
71 set.seed(123)
72 kmpp <- kmeanspp(Cars93[,c(5,7,12,14,19,22,25)],
73                      k = 3, start = "random", iter.max = 100, nstart = 1)
74 names(kmpp)
75 kmpp
76
77 ##### ClusterR package #####
78 # Gaussian mixture models, k-means, mini-batch-kmeans, k-medoids and
79 # affinity propagation clustering with the option to plot, validate,
80 # predict (new data) and estimate the optimal number of clusters.
81 install.packages("ClusterR")
82 library(ClusterR)
83 library(MASS)
84 data(Cars93)
85 kmrcpp <- KMeans_rcpp(Cars93[,c(5,7,12,14,19,22,25)],
86                         clusters = 3,
87                         num_init = 5, #異なる乱数で実行される計算回数
88                         max_iters = 100, seed = 123,
89                         initializer = "kmeans++")
90 #the method of initialization:optimal_init,quantile_init,kmeans++,random.
91 names(kmrcpp)
92 kmrcpp
93
94 #####Optimal_Clusters_KMeans()
95 kmopt <- Optimal_Clusters_KMeans(Cars93[,c(5,7,12,14,19,22,25)],
96                                     max_clusters=10,
97                                     criterion="distortion_fK",
98                                     plot_clusters=T)
99 kmopt
100
101 #####PAM K-medoids#####
102 #####kmeans:定量dataだけ、外れ値の影響大
103 #####Kmedoids:質的dataも可、外れ値の影響小
104 library(cluster)
105 plot(pam(Cars93[,c(5,7,12,14,19,22,25)],3),ask = T) #シルエットプロット
106 pamx <- pam(Cars93[,c(5,7,12,14,19,22,25)], 3)
107 summary(pamx)
108 plot(pamx)
109 pamx$medoids
110 pamx$clustering
111 pamx$clusinfo
112 pamx$silinfo
113 #####Data merge, CLdata保存
114 pam.cl <- factor(pamx$cluster)
115 write.csv(cbind(Cars93 , data.frame(pam.cl) ) ,
116           "data/cars93.pamcl.csv")
117
118

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